Chirality of wave functions for three coalescing levels

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Abstract

The coalescence of three levels has particular attractive features. Even though it may be difficult to realise such event in the laboratory (three additional real parameters must be adjusted), to take up the challenge seems worthwhile. In the same way as the chiral behaviour of a usual EP can give a direction on a line, the state vectors in the vicinity of an EP3 provide an orientation in the plane. The distinction between left and right handedness depends on the distribution of the widths of the three levels in the vicinity of the point of coalescence.

INTRODUCTION

There is substantial literature during the past decade relating to exceptional points [1], i.e. points where two eigenvalues of an operator coalesce giving rise to a square root singularity in the spectrum [2]. These singularities are generic and are thus encountered in virtually all physical problems associated with eigenvalues. They have been discussed in mechanical problems [3], in optics [4], for bound states [5] and resonances [6, 7] in quantum mechanics and in atomic physics [8]. The mutual influence of neighbouring exceptional points upon the phase behaviour of the associated wave functions is dealt with in [9]. Exceptional points also play a crucial role in quantum phase transitions [10]. Chiral behaviour of the eigenfunction [11] as well as effects of time reversal symmetry breaking is discussed in [12, 13]. Experimental manifestations including chiral behaviour have been achieved with microwave cavities [14] and coupled oscillators in electronic circuits [15]. A recent more mathematical exposé investigates exceptional points in the context of projective Hilbert spaces [16] while a connection to $\mathcal{PT}$ symmetric Hamilton operators [17] is found in [18]. In fact, it is established in [19] that, for a pseudohermitian $\mathcal{PT}$ symmetric Hamiltonian, the onset of spontaneous symmetry breaking by the wave function happens just at an exceptional point.

In many of the papers quoted above the notation EP was used denoting the generic exceptional point where two levels coalesce at a square root branch point. To distinguish it from the non-generic coalescence of three levels being the subject of the present paper we'll denote the generic EP by EP2 and we denote by EP3 the specific situation where three levels coalesce. We note that EPs of higher order have been implicitly encountered as the coalescence of two or more EP2 in a recent investigation of a complex WKB analysis [20].

THREE LEVELS COALESCING

The situation of three or more levels coalescing does not seem to have been investigated in great detail, the reason being that there are too many parameters needed to enforce such higher order coalescence. In fact, while two real parameters (one complex parameter) suffice to invoke the coalescence of two levels, for N levels coalescing $(N^2+N-2)/2$ real parameters are needed considering complex symmetric matrices. For $N=3$ it means that three additional real parameters have to be chosen judiciously to invoke the coalescence

of three levels in the complex plane of some complex parameter. Since, as seen below, the coalescence of just three levels has particular attractive features – for the coordinate systems used conventionally a distinction between left and right seems possible – the challenge to implement an experimental arrangement may just fall within reach of realisation.

We recall that the wave function at a usual EP2 has – for complex symmetric matrices – a fixed phase relationship of its components [14] that can be interpreted as a form of chirality [11]. Considering two coupled dissipative oscillators a particular EP2 specifies uniquely which of the two oscillators is leading by the phase $\pi/2$. In this particular mode, that is at the EP2, the two oscillators thus specify an orientation in one-dimensional space by simply placing them on a line and using the convention that an arrow points from the oscillator with the leading to the one with the lagging phase [15].

When three levels are coalescing the structure becomes much richer in comparison with an EP2, yet much of the structure turns out to be generalisations that could have been expected in hindsight. Of course, the simplest form of an operator giving rise to three levels coalescing is a three-dimensional matrix. Let us assume that any triple of the parameters in

$$H_0 = \begin{pmatrix} e1 & 0 & 0 \\ 0 & e2 & 0 \\ 0 & 0 & e3 \end{pmatrix} \quad \text{and} \quad H_1 = U \begin{pmatrix} o1 & 0 & 0 \\ 0 & o2 & 0 \\ 0 & 0 & o3 \end{pmatrix} U^T, \tag{1}$$

- with U a general three dimensional orthogonal matrix parametrised by three angles -, is so chosen that the full problem

$$H_0 + \lambda H_1 \tag{2}$$

has an EP3. If the parameters are all real (except for λ) such EP3 will occur at complex conjugate values of λ. Denoting such point by λ_c, the three levels are connected by a third root branch point (see appendix) and there exists the expansion:

$$E_j(\lambda) = E_c + \sum_{k=1}^{\infty} a_k (\sqrt[3]{\lambda - \lambda_c})^k \tag{3}$$

where the label $j = 1, 2, 3$ is specified by the first, second or third Riemann sheet of the third root in the λ-plane. As a consequence, for small values of $|\lambda - \lambda_c|$ the three complex energies $E_i(\lambda)$ form an equilateral triangle in the energy plane. The orientation of the triangle depends on $\arg(\lambda - \lambda_c)$ and on the parameters of the specific problem (1), which determine the complex value a_1 in (3). Generically we can order the energies according

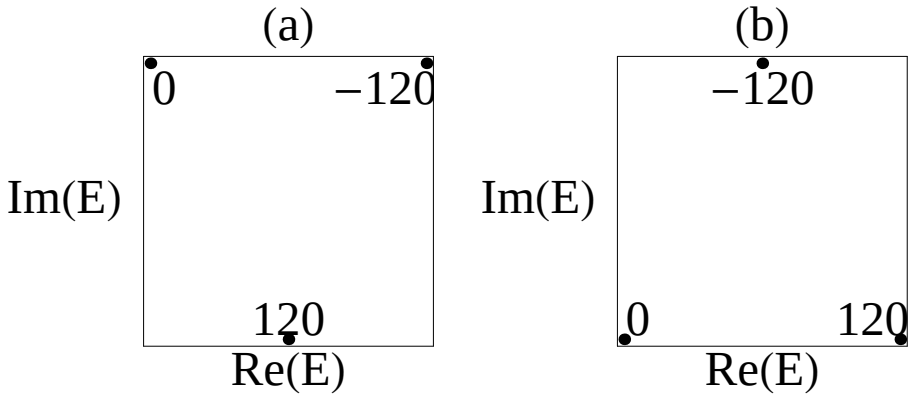

FIG. 1: The two basic positions of the three levels for small $|\lambda - \lambda_c|$ in the lower energy plane. The drawing is schematic in that the imaginary parts of two energies are equal: tilting either drawing by less than 30^0 still represents the specific case as discussed in the text. The lagging (120) and leading (-120) phases of the respective wave functions are indicated relative to the most left point (smallest $\Re(E)$, denoted E_1 in the main text). The EP3 lies in the centre of the equilateral triangles.

to their real parts, that is $\Re(E_1) < \Re(E_2) < \Re(E_3)$ (we dismiss the possibility that two real parts are equal as non-generic). There are two basic groups of orientation, depicted schematically in Fig.1: in (a) $\Im(E_2)$ is smaller than the imaginary parts of the other two energies - in other words it has the largest width - (recall that the energies all have negative imaginary parts), whereas in (b) $\Im(E_2)$ has the largest imaginary part (smallest width).

Now we turn to the eigenfunctions. It is three eigenfunctions that become aligned when approaching the EP3. There are the expansions

$$|\psi_j(\lambda)\rangle = |\psi_{EP3}\rangle + \sum_{k=1} (\sqrt[3]{\lambda - \lambda_c})^k |\phi_k\rangle. \tag{4}$$

Note that, as in (3), the label $j = 1, 2, 3$ is again specified by the Riemann sheet of the third root. For any $\lambda \neq \lambda_c$ the eigenfunctions form the usual bi-orthogonal complete system, *viz.*

$$\langle \tilde{\psi}_i(\lambda) | \psi_j(\lambda) \rangle \;=\; N_j(\lambda) \delta_{i,j} \tag{5}$$

$$\sum_j \frac{|\psi_j(\lambda)\rangle \langle \tilde{\psi}_j(\lambda)}{\langle \tilde{\psi}_j(\lambda) | \psi_j(\lambda) \rangle} \;=\; I. \tag{6}$$

It can be shown (see appendix) that the scalar product (5) vanishes as

$$N_j(\lambda) \sim \zeta \cdot (\lambda - \lambda_c)^{\frac{2}{3}} \quad \text{for} \quad \lambda \to \lambda_c \tag{7}$$

and similarly

$$\langle \tilde{\psi}_j(\lambda) | \psi_{EP3} \rangle \sim \eta \cdot (\lambda - \lambda_c)^{\frac{2}{3}} \quad \text{for} \quad \lambda \to \lambda_c \tag{8}$$

with some constants ζ, η being independent of j.

It should be noted that the structure of the eigenvectors at an EP3 is slightly more involved as there are three vectors that coalesce into $|\psi_{EP3}\rangle$ when $\lambda \to \lambda_c$. In view of the result (8) the expansion (4) implies that not only is

$$\langle\tilde{\psi}_{EP3}|\psi_{EP3}\rangle = 0$$

but also

$$\langle\tilde{\psi}_{EP3}|\phi_1\rangle = 0$$

where $|\phi_1\rangle$ occurs in the first order term in (4).

As a consequence, and in contrast to an EP2, the eigenfunction itself does not *a priory* bear a specific chiral phase structure at an EP3. It is rather in its immediate neighbourhood where the chiral phase structure is revealed. Similar to the reasoning in [11] an expansion of $|\psi_{EP}\rangle$ in terms of the normalised basis

$$|\chi_j(\lambda)\rangle = \frac{|\psi_j(\lambda)\rangle}{\sqrt{\langle\tilde{\psi}_j(\lambda)|\psi_j(\lambda)\rangle}} \tag{9}$$

yields the proper phase relation. Indeed, while it always possible for $\lambda \neq \lambda_c$ to write

$$|\psi_{EP3}\rangle = \sum_{j=1}^{3} c_j(\lambda)\chi_j(\lambda) \tag{10}$$

identically in λ, it is in particular for $\lambda \sim \lambda_c$

$$\begin{pmatrix} c_1(\lambda) \\ c_2(\lambda) \\ c_3(\lambda) \end{pmatrix} \sim \xi \sqrt[3]{|\lambda - \lambda_c|} \begin{pmatrix} e^{2i\pi j_1/3} \\ e^{2i\pi j_2/3} \\ e^{2i\pi j_3/3} \end{pmatrix} \tag{11}$$

with j_1, j_2, j_3 being a fixed permutation of $0, 1, 2$ specified below and ξ a complex constant. Recall that the normalised state vectors $\chi_j(\lambda)$ blow up as $1/\sqrt[3]{\lambda - \lambda_c}$ thus yielding a finite expression for $|\psi_{EP3}\rangle$ in (10). The result is due to the analytic structure of the third root branch point and is thus independent of a particular basis. As for an EP2, the fixed phase relations between the eigenstates in the immediate vicinity of the EP3 are of significance. This result is of course related to (4), the appealing feature of (11) lies in its similarity with the situation for an EP2. Note, however, that for an EP2 the phase difference is $\pi/2$ while here it is $2\pi/3$. This means that, in contrast to the EP2, where only a fourfold loop around

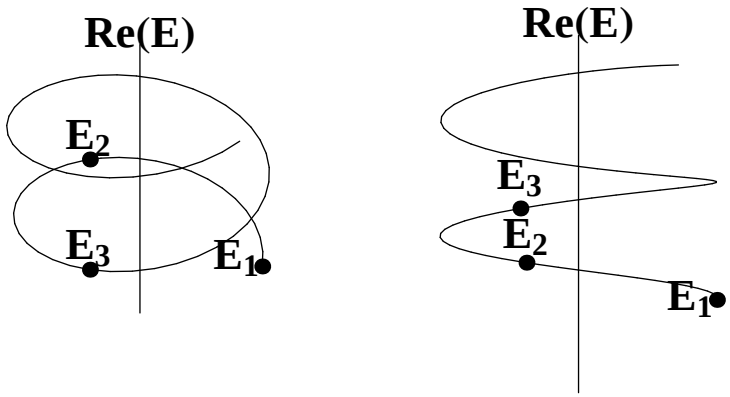

FIG. 2: Two perspective views of the three dimensional helix when the width of E_2 is larger than the other two. The coordinates of the points denoted by E_k are $(\cos(\Phi_k), \sin(\Phi_k), \Re(E_k))$ with $\Phi_{1,2,3} = (0^0, 120^0, 240^0)$.

the singularity restores the eigenfunctions, for the EP3 the eigenvectors are retrieved after three loops in the λ-plane just like for the corresponding energies.

The interesting question is now the precise association of the phases of the eigenfunctions with the complex values of the energies, that is with the frequencies and their widths. This association is illustrated in Fig.1. Choosing as reference point the eigenvector of the energy with smallest real part (frequency), then the eigenstate of the next frequency has a lagging phase of 120^0 if (and only if) the width is larger than the other two; the phase of the eigenstate with largest frequency would then be leading by 120^0. In turn, if the width of the middle frequency is smallest, the role of leading and lagging phase is swapped among the two states with the larger frequencies. This result is demonstrated below in a specific setting and confirmed numerically in numerous general examples.

The strict phase relations associated with the positions of the frequencies and widths of the three levels allows the interpretation of clear distinction between a left hand and a right hand helix. Fig.2 illustrates how a particular right handed helix is generated: in a three dimensional coordinate system the points $(\cos(\Phi_k), \sin(\Phi_k), \Re(E_k))$ with $\Phi_{1,2,3} = (0^0, 120^0, 240^0)$ invoke an oriented helix. The example refers to the case where the width of the middle frequency is largest, it generates a right handed helix. In turn, if the width of the middle frequency is smallest, the helix will be left handed.

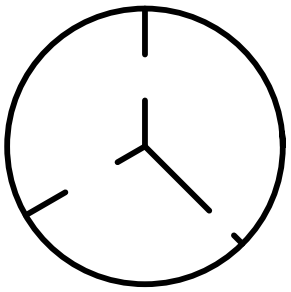

FIG. 3: Suggested arrangement, arbitrarily chosen, of a microwave cavity to invoke a threefold coalescence of levels. As for an EP2 the opening of the gaps and some Teflon piece in one or two of the chambers can be used as parameters to steer the system into an EP3. To avoid systematic degeneracies of the levels there should be no symmetry in the geometry of the cavity.

SPECIAL SETTING

The all important question is: can a threefold coalescence be arranged in the laboratory and are the energies and phases amenable to measurement? One suggestion could be a setting similar in spirit to the microwave experiment for an EP2. I could imagine a setup as illustrated in Fig.3. Again, this can be simulated by the simple matrix

$$H = \begin{pmatrix} e_1 & s1 & s3 \\ s1 & e_2 & s2 \\ s3 & s2 & e_3 \end{pmatrix} \tag{12}$$

where the s_j give the couplings (gaps in Fig.3) and the e_j are the (complex) energies. To facilitate matters, we consider in particular the problem

$$H_0 + s1\, H_1 = \begin{pmatrix} e_1 & 0 & s3 \\ 0 & e_2 & s2 \\ s3 & s2 & e_3 \end{pmatrix} + \lambda \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{13}$$

and choose the couplings s_2 and s_3 such that H_0 has a threefold coalescence. The choice

$$\begin{aligned} s2 &= \pm\sqrt{-\frac{(e_1 - 2e_2 + e_3)^3}{27(e_1 - e_2)}} \\ s3 &= \pm\sqrt{+\frac{(-2e_1 + e_2 + e_3)^3}{27(e_1 - e_2)}} \end{aligned} \tag{14}$$

achieves this goal with

$$E_c^{(1,2,3)} = \frac{1}{3}(e_1 + e_2 + e_3).$$

The perturbation by λ splits the coalescence into three levels and we obtain to lowest order (with $\lambda_c = 0$)

$$\begin{aligned} E_j = E_c \; + \; & \frac{2^{1/3}\sqrt{-(-2e_1+e_2+e_3)(e_1-2e_2+e_3)}}{3(e_1-e_2)^{1/3}} \sqrt[3]{|\lambda-\lambda_c|}\exp(2i(j-1)\pi/3) \\ + \; & O((\lambda-\lambda_c)^{4/3}) \end{aligned} \tag{15}$$

and, using the notation (4), the corresponding (unnormalised) eigenvectors are

$$|EP\rangle \; = \; \begin{pmatrix} \frac{\sqrt{-2e_1+e_2+e_3}}{\sqrt{3(e_1-e_2)}} \\ i\frac{\sqrt{e_1-2e_2+e_3}}{\sqrt{3(e_1-e_2)}} \\ 1 \end{pmatrix} \tag{16}$$

$$|\phi_1^j\rangle \; = \; \begin{pmatrix} i2^{1/3}\frac{\sqrt{e_1-2e_2+e_3}}{\sqrt{3}(e_1-e_2)^{5/6}} \\ -2^{1/3}\frac{\sqrt{-2e_1+e_2+e_3}}{\sqrt{3}(e_1-e_2)^{5/6}} \\ 0 \end{pmatrix} \exp(2i(j-1)\pi/3), \quad j=1,2,3 \tag{17}$$

and similar algebraic expressions for the higher orders.

The essential point here is the fact that - to lowest order - the three complex eigenvectors $|\phi_1^j\rangle$ differ only by a well defined phase; the precise specification of the particular eigenvector including its all important phase is given by its association with the levels E_j as indicated in Fig.1: the width of the second energy of the ordered frequencies characterises the orientation of the phases $\exp(2ij\pi/3)$; if $\Im E_2$ is smallest or largest a left or right hand helix is obtained, respectively.

CONCLUSION

A measurement of all three frequencies and their associated widths will thus predict the phase of the wave function in the immediate vicinity of the EP3. We recall that the single eigenstate $|\psi_{EP3}\rangle$ does not bear such information. The relevant phases sit in the part of the eigenstate that is switched on when moving away from the EP3 in the λ-plane. An experimental verification of this subtle behaviour would thus lead to a clear chiral characterisation in three dimensional space. We stress that there is no *a priory* handedness in a setting as

suggested for instance by Fig.3, neither is there any involvement of weak interaction. There is, however, the direction of time that specifies the various widths of a dissipative system. In other words, we here suggest that the arrow of time can invoke chirality.

ACKNOWLEDGEMENT

The author gratefully acknowledges constructive comments from all colleagues working at microwave cavity experiments at the TU Darmstadt.

APPENDIX

For an N-fold coalescence of eiegnvalues the N levels are connected by a branch point of N-th order. This follows from the fact that - for an N-dimensional matrix of the form $H_\lambda = H_0 + \lambda H_1$ - the determinant of $|H_\lambda - IE|$ vanishes linearly in the variable λ while the requirement of N coalescing levels entails an N-fold vanishing in the variable E, that is the following set of equations is to be satisfied simultaneously

$$\frac{\mathrm{d}^k}{\mathrm{d}E^k}|H_\lambda - IE| = 0, \quad k = 0, \ldots, N-1.$$

This is possible only if

$$E(\lambda) = E_c + \sum_{m=1}^{\infty} c_m (\sqrt[N]{\lambda - \lambda_c})^m.$$

Here the N eigenvalues are given by the values upon the N sheets of the N-th root.

The N eigenstates coalesce likewise into one eigenvector. There is the expansion

$$|\psi(\lambda)\rangle = |\psi_{EP\,N}\rangle + \sum_{m=1}^{\infty} |\phi_m\rangle (\sqrt[N]{\lambda - \lambda_c})^m.$$

Note, however, that for the scalar product the following behaviour prevails

$$\langle\psi(\lambda)|\psi_{EP\,N}\rangle \sim (\lambda - \lambda_c)^{\frac{N-1}{N}}$$

as follows from considering

$$\begin{aligned}(E(\lambda)) - E_c)\langle\psi(\lambda)|\psi_{EP\,N}\rangle &= \langle\psi(\lambda)|H_\lambda - H_{\lambda_c}|\psi_{EP\,N}\rangle \\ &= (\lambda - \lambda_c)\langle\psi(\lambda)|H_1|\psi_{EP\,N}\rangle.\end{aligned}$$

The right hand side vanishes linearly when $\lambda \to \lambda_c$ while $(E(\lambda)) - E_c) \sim \sqrt[N]{\lambda - \lambda_c}$. Note that these analytic properties imply the relations

$$\langle \psi_{EP\,N} | \phi_m \rangle = 0 \quad \text{for} \quad m = 1, \ldots, N-1$$

and

$$\langle \phi_m | \phi_{m'} \rangle = 0 \quad \text{for} \quad m + m' \leq N - 2.$$

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